Structures of Er in Oxygen-free Si

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Er-doped Si had been considered the simplest 1.54-μm-luminescent system for Si integration, but the low solubility of Er has made its use impractical. Basic materials-design issues require understanding the reasons for such low solubility.

Arguments of Er bond strengths and chemical behavior (used this year for explaining the high solubility of Er in GaN) were extended to Si, indicating that sites for substitutional/interstitial occupation by Er (i.e., point defects) are not possible but sites resembling those in bulk-like $ErSi_{2-x}$ (i.e., extended defects) are. New x-ray absorption data from both implanted and MBE-deposited Er in Si, along with new LDA calculations, conclusively support the picture that Er —when in Si— assumes a large metal-atom (rather than a small ionic) electronic configuration, which is stabilized by neighboring Er atoms in a silicide-like structure.